

SHARP TWO-SIDED HEAT KERNEL ESTIMATES OF TWISTED TUBES AND APPLICATIONS

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ABSTRACT. We prove on-diagonal bounds for the heat kernel of the Dirichlet Laplacian $-\Delta_\Omega^D$ in locally twisted three-dimensional tubes Ω . In particular, we show that for any fixed x the heat kernel decays for large times as $e^{-E_1 t} t^{-3/2}$, where E_1 is the fundamental eigenvalue of the Dirichlet Laplacian on the cross section of the tube. This shows that any, suitably regular, local twisting speeds up the decay of the heat kernel with respect to the case of straight (untwisted) tubes. Moreover, the above large time decay is valid for a wide class of subcritical operators defined on a straight tube. We also discuss some applications of this result, such as Sobolev inequalities and spectral estimates for Schrödinger operators $-\Delta_\Omega^D - V$.

1. Introduction

Let $\omega \subset \mathbb{R}^2$ be an open bounded set and let $\Omega_0 = \omega \times \mathbb{R}$ be a straight tube in \mathbb{R}^3 . By separation of variables it is easy to see that the heat kernel of the Dirichlet Laplacian $-\Delta_{\Omega_0}^D$ on Ω_0 satisfies

$$k(t, x, y) := e^{tE_1} e^{t\Delta_{\Omega_0}^D}(x, y) \sim t^{-\frac{1}{2}} \quad \text{as } t \rightarrow \infty, \quad (1.1)$$

where E_1 is the principal eigenvalue of $-\Delta_\omega^D$, the Dirichlet Laplacian on ω . Let us now define the twisted tube Ω by

$$\Omega = \{r_\theta(x_3)x \mid x = (x_1, x_2, x_3) \in \Omega_0\},$$

where

$$r_\theta(x_3) = \begin{pmatrix} \cos \theta(x_3) & \sin \theta(x_3) & 0 \\ -\sin \theta(x_3) & \cos \theta(x_3) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and $\theta : \mathbb{R} \rightarrow \mathbb{R}$ is the angle of rotation. Here and in the sequel we will denote by x the variable in the straight tube Ω_0 and by \mathbf{x} the variable in the twisted tube Ω . We assume that the support of $\dot{\theta}$, the derivative of θ , is compact, see Section 2 for more details. It then follows that the spectrum of $-\Delta_\Omega^D$ coincides with the half-line $[E_1, \infty)$. Therefore, it is convenient to work with the shifted operator $-\Delta_\Omega^D - E_1$. This is a nonnegative self-adjoint operator which generates a contraction, positivity preserving semigroup $e^{t(\Delta_\Omega^D + E_1)}$ on $L^2(\Omega)$. The main object of our interest is its integral kernel

$$k(t, \mathbf{x}, \mathbf{y}) := e^{t(\Delta_\Omega^D + E_1)}(\mathbf{x}, \mathbf{y}), \quad \mathbf{x}, \mathbf{y} \in \Omega. \quad (1.2)$$

In particular, we are interested in the influence of twisting on the long time behavior of $k(t, \mathbf{x}, \mathbf{y})$. This is motivated by the fact that, under appropriate assumptions on ω and $\dot{\theta}$,

the Dirichlet Laplacian in the twisted tube Ω satisfies a Hardy-type inequality

$$-\Delta_{\Omega}^D - E_1 \geq \frac{c}{1 + \mathbf{x}_3^2} \quad (1.3)$$

in the sense of quadratic forms, see [EKK]. One of the consequences of this inequality is the existence of a finite positive (minimal) Green function of $-\Delta_{\Omega}^D - E_1$, see e.g. [Gr06, PT06]. Using a different terminology, the associated semigroup is transient. On the other hand, (1.1) implies that the associated semigroup of $-\Delta_{\Omega_0}^D - E_1$ corresponding to the straight tube is recurrent (see also [FOT]). In other words, inequality (1.3) implies that $\int_0^\infty k(t, \mathbf{x}, \mathbf{y}) dt < \infty$ for all $\mathbf{x} \neq \mathbf{y}$, while the recurrency of $-\Delta_{\Omega_0}^D - E_1$ means that $\int_0^\infty k(t, x, y) dt = \infty$. Moreover, since $k(t, \mathbf{x}, \mathbf{y})$ and $k(t, \mathbf{x}, \mathbf{x})$ are pointwise equivalent for all $t \geq 1$ [D97, Theorem 10], and since $k(t, \mathbf{x}, \mathbf{x})$ is nonincreasing in t it follows that

$$k(t, \mathbf{x}, \mathbf{x}) = o(t^{-1}) \quad \text{as } t \rightarrow \infty. \quad (1.4)$$

This means that the heat kernel of the twisted tube must decay faster to zero than the heat kernel of the straight tube given by (1.1). In fact, the validity of the Hardy inequality (1.3) can be viewed as a qualitative description of the improved decay of $k(t, \mathbf{x}, \mathbf{y})$, so that the present investigation of obtaining sharp quantitative bounds for $k(t, \mathbf{x}, \mathbf{y})$ is a natural continuation of [EKK].

The connection between twisting and the heat equation was pointed out for the first time in the recent paper of Krejčířík and Zuazua [KZ10]. Let $L^2(\Omega, K)$ be the weighted L^2 space, with the weight $K(x) = e^{\mathbf{x}_3^2/4}$. The authors of [KZ10] proved that

$$\|e^{t(\Delta_{\Omega}^D + E_1)}\|_{L^2(\Omega, K) \rightarrow L^2(\Omega)} \leq C(1+t)^{-\frac{a}{2}} \quad \forall t \geq 0, \quad (1.5)$$

where $C > 0$ and $a \geq 3/2$: notice that a would be equal to $1/2$ in a straight tube. Similar result was obtained by the same authors in [KZ11] for the heat semigroup of the twisted Dirichlet-Neumann waveguide. From the applicative point of view, we mention that it is known that twisting enhances heat transfer, see for example [B, MB]. This phenomenon seems to be utilized in the so called Twisted Tube technology.

The aim of this paper is to establish sharp pointwise on-diagonal heat kernel estimates. In fact, as one of our main results we will show that

$$k(t, \mathbf{x}, \mathbf{x}) \asymp \frac{\text{dist}(\mathbf{x}, \partial\Omega)^2}{\sqrt{t}} \min \left\{ \frac{1 + \mathbf{x}_3^2}{t}, 1 \right\}, \quad \forall t \geq 1, \quad (1.6)$$

see Theorem 3.1. Such a two-sided pointwise bound on the heat kernel of course gives us a more detailed information than an integral bound. Moreover, a simple application of (1.6) allows us to extend inequality (1.5) to a wider class of subspaces of $L^2(\Omega)$ and also to corresponding subspaces of $L^1(\Omega)$, see Theorem 4.4.

The proof of estimate (1.6) relies on the study of positive global solutions of the equation $(-\Delta_{\Omega}^D - E_1)u = 0$ in Ω and of suitable functional inequalities on the corresponding weighted L^2 spaces. We would like to point out that the Hardy inequality (1.3) is used only implicitly, to ensure the subcriticality of $-\Delta_{\Omega}^D - E_1$. Since heat kernel estimates can be reformulated in probabilistic terms in term of the survival probability of the Brownian bridge killed upon exiting Ω , our results also imply sharp bounds for such probability: roughly speaking, the $t^{-3/2}$ decay of the kernel for a fixed \mathbf{x} might be expressed by saying that the longitudinal part of the Brownian bridge sees, asymptotically as $t \rightarrow \infty$, the twist as if it were a Dirichlet

boundary condition imposed on the cross-section of the tube. Hence the corresponding heat kernel resembles the one generated by the Dirichlet Laplacian on a half-line.

As applications of our heat kernel estimates we prove a family of Sobolev-type inequalities for the operator $-\Delta_\Omega^D - E_1$, see Theorem 5.4, and an upper bound on the number of eigenvalues of Schrödinger operators $-\Delta_\Omega^D - V$, where V is an additional electric potential, Theorem 5.1. Both these results fail in straight tubes.

While the behavior of the Dirichlet heat kernel on bounded Euclidean regions is well understood (see e.g. [D87], [Zh02] and references therein), much less is known in unbounded regions because of the great variety of possible geometrical situations. In fact, a rather complete study is available, as far as we know, only in exterior domains, namely in domains of the form A^c , A being a compact set with nonempty interior: see [GS] (and [CMS] for some particular cases) for its behavior both in the transient and in the recurrent case when in addition the spatial variables are required to be not too close to the boundary, and [Zh03] for the remaining range, at least in the transient case. See also [DB] and references quoted therein for the study of heat kernel behavior in other special classes of unbounded domains. Note also that the behavior of the heat kernel for $t \leq 1$ in the class of domains considered in this paper is entirely known from [Zh02]. We would like to mention that the fact that heat kernels of subcritical operators decay faster than heat kernels of suitably related critical operators has been proved in larger generality in [FKP], but the general situation studied there does not allow for quantitative statements.

Our results are not restricted only to twisted tubes. Indeed, if $L := -\nabla \cdot (a\nabla) + V$ is a uniformly elliptic operator with smooth enough coefficients which is defined on Ω_0 such that $L = -\Delta - E_1$ in $\{(x', x_3) \in \Omega_0 \mid |x_3| > R\}$, and L is subcritical in Ω_0 , then a straightforward application of our technique yields

$$\exp(-tL)(x, x) \asymp \frac{\text{dist}(x, \partial\Omega_0)^2}{\sqrt{t}} \min \left\{ \frac{1 + x_3^2}{t}, 1 \right\}, \quad \forall t \geq 1, \quad \forall x \in \Omega_0. \quad (1.7)$$

See Subsection 3.3 and in particular Theorem 3.18 for a more detailed discussion.

Let us briefly outline the content of the paper. In Section 2 we formulate our main assumptions on ω and θ and fix some necessary notation. The crucial heat kernel upper bound is proven in Section 3.1, see Theorem 3.12. The central idea of the proof is to establish suitable generalized Nash inequalities on carefully chosen weighted L^2 spaces and to use the equivalence between such inequalities and ultracontractivity estimates, cf. [Cou]. Off-diagonal upper bound are then a straightforward consequence of [Gr97]. In Section 3.2 we prove the lower bound in (1.6) by means of a Dirichlet bracketing argument. Improvements of inequality (1.5) for a larger class of data, including optimal L^1 and L^∞ versions, are given in Section 4. In the closing Section 5 we prove spectral estimates for Schrödinger operators on Ω and a family of Hardy-Sobolev type inequalities for functions from $H_0^1(\Omega)$ (cf. [PT09]). The latter are, similarly as the Hardy inequality (1.3), yet another example of functional inequalities induced by twisting; i.e. they fail in the straight tube Ω_0 .

2. Preliminaries

Throughout the paper we will work under the following hypotheses on ω and θ :

Assumption 2.1. ω is an open bounded connected subset of \mathbb{R}^2 with a C^2 -regular boundary which contains the origin. Moreover, ω is not a disc or a ring centered at the origin.

Assumption 2.2. The function θ belongs to the class $C^{2,\alpha}(\mathbb{R})$ with some $\alpha > 0$ and the support of $\dot{\theta}$ is compact. Without loss of generality we assume that $\theta(x_3) = 0$ for all $x_3 < \inf \text{supp } \dot{\theta}$.

Under these assumptions we define the Dirichlet Laplacian $-\Delta_\Omega^D$ as the unique self-adjoint operator in $L^2(\Omega)$ generated by the closed quadratic form

$$\int_\Omega |\nabla u|^2 d\mathbf{x} \quad u \in H_0^1(\Omega). \quad (2.1)$$

As for the notation, given a set M and functions $f_1, f_2 : M \rightarrow \mathbb{R}_+$ we will use the convention

$$f_1(z) \asymp f_2(z) \iff \exists c > 0 : \forall z \in M \quad c^{-1}f_1(z) \leq f_2(z) \leq cf_1(z).$$

Moreover, given a measure $d\mu(x) = \mu(x) dx$ on Ω_0 and $p \geq 1$, we denote by $L^p(\Omega_0, \mu)$ the corresponding L^p space with respect to $d\mu$. The same notation will be used for the Sobolev spaces H^1 and H_0^1 . A point $x \in \Omega_0$ will be denoted by $x = (x', x_3)$, where $x' \in \omega$ and $x_3 \in \mathbb{R}$. Set

$$\omega_a := \{(x', x_3) \in \Omega_0 \mid x_3 = a\}.$$

We will also need the functions

$$\gamma(t) := \begin{cases} t^{-5/2}, & 0 < t \leq 1, \\ t^{-3/2}, & 1 < t < \infty, \end{cases} \quad \Gamma(t) := \begin{cases} t^{-5/2}, & 0 < t \leq 1, \\ t^{-1/2}, & 1 < t < \infty. \end{cases} \quad (2.2)$$

By the symbol c we will denote a generic positive constant whose value might change from line to line. Finally, we introduce the distance function

$$\rho(\mathbf{x}) := \text{dist}(\mathbf{x}, \partial\Omega), \quad \mathbf{x} \in \Omega.$$

We have the following auxiliary result.

Lemma 2.3. *Let ψ_1 be the normalized principal eigenfunction of $-\Delta_\omega^D$ associated to E_1 . Let $T_\theta : \Omega \rightarrow \omega$ be defined by*

$$T_\theta(\mathbf{x}) = (\cos \theta(\mathbf{x}_3) \mathbf{x}_1 - \sin \theta(\mathbf{x}_3) \mathbf{x}_2, \sin \theta(\mathbf{x}_3) \mathbf{x}_1 + \cos \theta(\mathbf{x}_3) \mathbf{x}_2).$$

Then $\psi_1(T_\theta(\mathbf{x})) \asymp \rho(\mathbf{x})$.

Proof. Let $\Omega_{\mathbf{x}} = \{\mathbf{y} \in \Omega : \mathbf{y}_3 = \mathbf{x}_3\}$ and define $\tilde{\rho}(\mathbf{x}) = \text{dist}(\mathbf{x}, \Omega_{\mathbf{x}})$. Since the boundary of ω is C^2 -smooth, the Hopf boundary point lemma, cf. [D89, Sect.4.6], implies that $\psi_1(T_\theta(\mathbf{x})) \asymp \tilde{\rho}(\mathbf{x})$. On the other hand, from the regularity assumptions on θ it follows that $\tilde{\rho}(\mathbf{x}) \asymp \rho(\mathbf{x})$. \square

3. Heat kernel bounds

The main result of this section is the following

Theorem 3.1. *There exists a constant $c > 0$ such that for any $\mathbf{x} \in \Omega$ and any $t \geq 1$ we have*

$$c^{-1} \frac{\rho^2(\mathbf{x})}{\sqrt{t}} \min \left\{ \frac{1 + \mathbf{x}_3^2}{t}, 1 \right\} \leq k(t, \mathbf{x}, \mathbf{x}) \leq c \frac{\rho^2(\mathbf{x})}{\sqrt{t}} \min \left\{ \frac{1 + \mathbf{x}_3^2}{t}, 1 \right\}. \quad (3.1)$$

Remark 3.2. Note that while $k(t, \mathbf{x}, \mathbf{x}) \asymp t^{-3/2}$ as $t \rightarrow \infty$ holds pointwise for any $\mathbf{x} \in \Omega$, we have $\sup_{\mathbf{x}} k(t, \mathbf{x}, \mathbf{x}) \asymp t^{-1/2}$ as $t \rightarrow \infty$. Similar discrepancy between the behavior of $k(t, \mathbf{x}, \mathbf{x})$ and $\sup_{\mathbf{x}} k(t, \mathbf{x}, \mathbf{x})$ has been observed, for example, also in [D97].

Remark 3.3. The behavior of $k(t, \mathbf{x}, \mathbf{y})$ for small times is known and, as expected, is independent of twisting. The following two-sided estimate is due to [Zh02]:

$$\forall t \leq 1 : \quad c^{-1} \min \left\{ \frac{\rho^2(\mathbf{x})}{t}, 1 \right\} t^{-\frac{3}{2}} \leq k(t, \mathbf{x}, \mathbf{x}) \leq c \min \left\{ \frac{\rho^2(\mathbf{x})}{t}, 1 \right\} t^{-\frac{3}{2}}, \quad (3.2)$$

see also [D87].

Theorem 3.1 will be proven in several steps in the following two subsections.

3.1. Heat kernel upper bounds. We introduce the transformation

$$(U_\theta \varphi)(x) := \varphi(r_\theta(x_3)x), \quad x \in \Omega_0, \quad \varphi \in L^2(\Omega),$$

which maps $L^2(\Omega)$ unitarily onto $L^2(\Omega_0)$. A straightforward calculation then shows that $H = U_\theta(-\Delta_\Omega^D)U_\theta^{-1}$ is the self-adjoint operator in $L^2(\Omega_0)$ which acts on its domain as

$$H := -\Delta_\omega^D - (\partial_3 + \dot{\theta}(x_3)\partial_\tau)^2, \quad (3.3)$$

where $\partial_\tau := x_1\partial_2 - x_2\partial_1$. The shifted Laplacian $-\Delta_\Omega^D - E_1$ transforms accordingly into the operator

$$H_\theta := H - E_1 = U_\theta(-\Delta_\Omega^D - E_1)U_\theta^{-1}, \quad \text{in } L^2(\Omega_0)$$

which is generated by the quadratic form

$$\mathcal{Q}[u] := \int_{\Omega_0} \left(|\nabla_\top u|^2 + |\partial_3 u + \dot{\theta}\partial_\tau u|^2 - E_1|u|^2 \right) dx, \quad u \in D(\mathcal{Q}) = H_0^1(\Omega_0), \quad (3.4)$$

where $\nabla_\top := (\partial_1, \partial_2)$.

We will also consider the reference operator

$$A := -\Delta_{\Omega_0}^D + \dot{\theta}^2(x_3) - E_1 \quad \text{in } L^2(\Omega_0) \quad (3.5)$$

with Dirichlet boundary conditions at $\partial\Omega_0$. Recall the Hardy-type inequality

$$\int_{\Omega_0} \left(|\nabla_\top u|^2 + |\partial_3 u + \dot{\theta}\partial_\tau u|^2 - E_1|u|^2 \right) dx \geq c_h \int_{\Omega_0} \dot{\theta}^2 |u|^2 dx, \quad \forall u \in H_0^1(\Omega_0), \quad (3.6)$$

where the constant $c_h > 0$ depends on $\dot{\theta}$ and ω but not on u , see [EKK]. In the language of criticality theory this inequality says that H_θ is a subcritical operator (see for example [PT06]). On the other hand, since $-\Delta_{\Omega_0}^D \geq E_1$, it follows from the definition of the operator A that

$$A \geq \dot{\theta}^2.$$

Hence A itself is a subcritical operator. We denote the minimal positive Green functions of H_θ and A by $G_\theta(x, y)$ and $G_A(x, y)$, respectively. The following theorem plays a crucial role in the proof of our heat kernel upper bounds.

Theorem 3.4. *Let H_1 and H_2 be two subcritical operators in the tube Ω_0 such that $H_1 = H_2$ in $\{(x', x_3) \in \Omega_0 \mid |x_3| > R\}$, and let $G_k(x, y)$ be the positive minimal Green function of H_k in Ω_0 , $k = 1, 2$. Assume that the coefficients of H_1 and H_2 are Hölder continuous in $\{(x', x_3) \in \overline{\Omega_0} \mid |x_3| < R + 6\}$. Then*

$$G_1 \asymp G_2 \quad \text{in } \Omega_0 \times \Omega_0 \setminus \{(x, x) \mid x \in \Omega_0\}. \quad (3.7)$$

In particular, there exists a positive constant C such that

$$C^{-1} G_\theta(x, y) \leq G_A(x, y) \leq C G_\theta(x, y) \quad (3.8)$$

for all $x, y \in \Omega_0$.

Proof. Without loss of generality, we may assume that $H_1 = H_2$ in $\{(x', x_3) \in \Omega_0 \mid |x_3| > 1\}$. By the interior Harnack inequality for H_k^* , the formal adjoint of H_k and the behavior of the Green functions near the singular point we have that $G_1(0, (0, 0, \pm 2)) \asymp G_2(0, (0, 0, \pm 2))$. Hence, the Harnack boundary principle for $H_1^* = H_2^*$ [A78, CFMS] implies that

$$G_1(0, y) \asymp G_2(0, y) \quad \forall y \in \omega_{\pm 2}. \quad (3.9)$$

Since $G_k(0, y)$ has minimal growth at infinity of $\{y = (y', \eta) \in \partial\Omega_0 \mid \eta > 2\}$ and $\{y = (y', \eta) \in \partial\Omega_0 \mid \eta < -2\}$ it follows from (3.9)

$$G_1(0, y) \asymp G_2(0, y) \quad \forall y \in \omega_\eta, \quad |\eta| > 2. \quad (3.10)$$

Now, fix $y \in \omega_\eta$, $|\eta| > 3$. Without loss of generality, we may assume $\eta > 3$. Then by the Harnack boundary principle for $H_1 = H_2$ we have

$$\frac{G_1(x, y)}{G_1((0, 0, \pm 2), y)} \asymp \frac{G_2(x, y)}{G_2((0, 0, \pm 2), y)} \quad \forall x \in \omega_{\pm 2}, \forall y \in \omega_\eta, \quad |\eta| > 3. \quad (3.11)$$

Recall that by the interior Harnack inequality for H_k we have $G_k((0, 0, \pm 2), y) \asymp G_k(0, y)$. Hence, it follows from (3.11) that

$$\frac{G_1(x, y)}{G_1(0, y)} \asymp \frac{G_2(x, y)}{G_2(0, y)} \quad \forall x \in \omega_{\pm 2}, \forall y \in \omega_\eta, \quad |\eta| > 3. \quad (3.12)$$

Combining (3.10) and (3.12) we obtain

$$G_1(x, y) \asymp G_2(x, y) \quad \forall x \in \omega_{\pm 2}, \quad \forall y \in \omega_\eta, \quad |\eta| > 3. \quad (3.13)$$

The minimality of $G_k(\cdot, y)$ in $\{(x', \xi) \in \partial\Omega_0 \mid \xi < -2\}$ and (3.13) imply

$$G_1(x, y) \asymp G_2(x, y) \quad \forall x \in \omega_\xi, \quad \xi < -2.$$

On the other hand, since $G_1(x, y) \asymp G_2(x, y)$ in a small punctured neighborhood of y (the size of the neighborhood depends on $\text{dist}(y, \partial\Omega_0)$), and in light of (3.13) and the minimality of G_k , we obtain that

$$G_1(x, y) \asymp G_2(x, y) \quad \forall x \in \omega_\xi, \quad \xi > 2.$$

So, we obtained

$$G_1(x, y) \asymp G_2(x, y) \quad \forall x \in \omega_\xi, \quad |\xi| \geq 2 \text{ and } \forall y \in \omega_\eta, \quad |\eta| \geq 3. \quad (3.14)$$

Denote by $G_k^{\Omega_N}(x, y)$ the positive minimal Green function of H_k in $\Omega_N := \omega \times (-N, N)$, $k = 1, 2$, $N \leq 6$. It is known (see for example [A97, HS]) that for a fixed N we have

$$G_1^{\Omega_N} \asymp G_2^{\Omega_N} \quad \text{in } \Omega_N \times \Omega_N \setminus \{(x, x) \mid x \in \Omega_N\}. \quad (3.15)$$

Fix $N = 5$. It follows from the boundary Harnack principle (in x) that for $k = 1, 2$ we have

$$\frac{G_k(x, y)}{G_k((0, 0, \xi), y)} \asymp \frac{G_k^{\Omega_5}(x, y)}{G_k^{\Omega_5}((0, 0, \xi), y)} \quad \forall x \in \omega_\xi, \xi = \pm 4, \forall y \in \omega_\eta, \quad |\eta| \leq 3. \quad (3.16)$$

On the other hand,

$$G_k((0, 0, \xi), 0) \asymp 1, \quad G_k^{\Omega_5}((0, 0, \xi), 0) \asymp 1 \quad \xi = \pm 4, \quad k = 1, 2.$$

Hence, the boundary Harnack principle (in y) implies that

$$G_k((0, 0, \xi), y) \asymp G_k^{\Omega_5}((0, 0, \xi), y) \quad \forall \xi = \pm 4, \forall y \in \omega_\eta, |\eta| \leq 3. \quad (3.17)$$

Consequently, (3.16), (3.17), the behavior of Green functions near the singularity, and the comparison principle imply that

$$G_k(x, y) \asymp G_k^{\Omega_5}(x, y) \quad \forall x \in \omega_\xi, |\xi| \leq 4, \forall y \in \omega_\eta, |\eta| \leq 3. \quad (3.18)$$

In light of (3.18) and (3.15) with $N = 5$ we obtain

$$G_1(x, y) \asymp G_2(x, y) \quad \forall x \in \omega_\xi, |\xi| \leq 4, \text{ and } \forall y \in \omega_\eta, |\eta| \leq 3. \quad (3.19)$$

Since G_k has minimal growth at infinity, it follows from (3.19) that

$$\begin{aligned} G_1(x, y) &\asymp G_2(x, y) \quad \text{if} \\ (x, y) &\in \{x \in \omega_\xi, |\xi| \geq 4; y \in \omega_\eta, |\eta| \leq 3\} \cup \{x \in \omega_\xi, |\xi| \leq 2; y \in \omega_\eta, |\eta| \geq 3\}. \end{aligned} \quad (3.20)$$

Thus, (3.14), (3.19), and (3.20) imply (3.7). \square

Remark 3.5. Let M be a noncompact smooth Riemannian manifold and let Ω and Ω_j , $j = 0, 1, \dots, \ell$ be subdomains of M with Lipschitz boundaries such that

$$\Omega = \bigcup_{j=0}^{\ell} \Omega_j, \quad \Omega_i \cap \Omega_j = \emptyset \quad \forall 1 \leq i < j \leq \ell,$$

and such that $\overline{\Omega_0}$ is compact in M . Let H_1 and H_2 be two subcritical operators in Ω such that $H_1 = H_2$ in $\bigcup_{j=1}^{\ell} \Omega_j$, and let $G_k(x, y)$ be the positive minimal Green function of H_k in Ω , $k = 1, 2$ (cf. [M90, Section 7]). Assume that the coefficients of H_1 and H_2 are Hölder continuous in $\overline{\Omega_0}$. By adopting the proof of Theorem 3.4 we obtain that

$$G_1 \asymp G_2 \quad \text{in } \Omega \times \Omega \setminus \{(x, x) \mid x \in \Omega\}.$$

The subcriticality of the operator $-\frac{d^2}{dr^2} + \dot{\theta}^2(r)$ on \mathbb{R} implies that there are exactly two positive minimal solutions (in the sense of Martin boundary) g_j , $j = 1, 2$ of the equation $(-\frac{d^2}{dr^2} + \dot{\theta}^2(r))g = 0$ in \mathbb{R} satisfying $g_j(0) = 1$ [M86, Appendix 1]. Moreover, we may assume that

$$g_1(x_3) \asymp 1 + \Theta(-x_3)|x_3|, \quad g_2(x_3) \asymp 1 + \Theta(x_3)|x_3|, \quad (3.21)$$

where Θ is the Heaviside function. Let

$$g_0 := (g_1 + g_2)/2. \quad (3.22)$$

Clearly, we have

$$g_0(x_3) \asymp 1 + |x_3|. \quad (3.23)$$

The functions $w_j : \Omega \rightarrow \mathbb{R}$ given by

$$w_j(x) := \psi_1(x_1, x_2) g_j(x_3), \quad j = 0, 1, 2, \quad (3.24)$$

then satisfy

$$Aw_j = 0, \quad w_j > 0 \quad \text{in } \Omega_0, \quad w_j = 0 \quad \text{on } \partial\Omega_0. \quad (3.25)$$

We note that for any positive solution w of the equation $Aw = 0$ on Ω_0 that vanishes on $\partial\Omega_0$ there exists a unique pair of nonnegative numbers α and β such that $w = \alpha w_1 + \beta w_2$ [M90, Theorem 7.1].

Next, we apply the above crucial results to obtain the following lemma.

Lemma 3.6. *There exist positive functions $v_j \in C^2(\Omega_0)$, $j = 0, 1, 2$, such that*

$$H_\theta v_j = 0, \quad v_j(x) \asymp w_j(x). \quad (3.26)$$

Proof. This follows from Theorem 3.4 and [P88, Lemma 2.4]. \square

With this result at hand, we define the transformation $\mathcal{U}_0 : L^2(\Omega_0) \rightarrow L^2(\Omega_0, v_0^2)$ by

$$(\mathcal{U}_0 u)(x) = v_0^{-1}(x) u(x), \quad x \in \Omega_0. \quad (3.27)$$

\mathcal{U}_0 maps $L^2(\Omega_0)$ unitarily onto $L^2(\Omega_0, v_0^2)$ and $\mathcal{Q}[u]$ transforms into the closed quadratic form

$$Q_0[f] := \mathcal{Q}[v_0 f] = \int_{\Omega_0} \left(|\nabla_\tau f|^2 + |\partial_3 f + \dot{\theta} \partial_\tau f|^2 \right) v_0^2 dx, \quad f \in D(Q_0) = H^1(\Omega_0, w_0^2). \quad (3.28)$$

The fact that the form domain $D(Q_0)$ coincides with $H^1(\Omega_0, w_0^2)$ follows from the regularity of ω , see [DS], and from the equivalence

$$c |\nabla f|^2 \leq |\nabla_\tau f|^2 + |\partial_3 f + \dot{\theta} \partial_\tau f|^2 \leq c^{-1} |\nabla f|^2.$$

The upper bound is immediate. The lower bound will be given in the proof of Proposition 3.9.

We denote by B_0 the self-adjoint operator in $L^2(\Omega_0, v_0^2)$ associated with the form $Q_0[f]$. By standard arguments, see e.g. [D89, Section 4.7], it follows that $\exp(-tB_0)$ is a symmetric submarkovian semigroup on $L^2(\Omega_0, v_0^2)$ and since

$$H_\theta = \mathcal{U}_0^{-1} B_0 \mathcal{U}_0,$$

we get

$$e^{-tH_\theta}(x, y) = v_0(x) v_0(y) e^{-tB_0}(x, y). \quad (3.29)$$

Let $\lambda > 1$ and introduce a C^1 decreasing bijection m_λ of \mathbb{R}_+ onto itself by

$$m_\lambda(t) := \lambda \begin{cases} t^{-5/2}, & 0 < t \leq 1/2, \\ \chi(t), & 1/2 < t \leq 1, \\ t^{-3/2}, & 1 < t < \infty, \end{cases} \quad (3.30)$$

where χ is a C^1 decreasing convex function chosen such that $m_\lambda(t)$ is $C^1(\mathbb{R}_+)$. Next we define

$$\xi_\lambda(r) := -m'_\lambda(m_\lambda^{-1}(r)), \quad r \in \mathbb{R}_+. \quad (3.31)$$

We have

Lemma 3.7. *There exists $\lambda_0 > 0$ such that the inequality*

$$\xi_\lambda(\|f\|_{L^2(\Omega_0, w_0^2)}^2) \leq \int_{\Omega_0} |\nabla f|^2 w_0^2 dx \quad (3.32)$$

holds for all $f \in H^1(\Omega_0, w_0^2) \cap L^1(\Omega_0, w_0^2)$ with $\|f\|_{L^1(\Omega_0, w_0^2)} \leq 1$ and all $\lambda > \lambda_0$.

Proof. Consider the heat kernel $e^{-tA}(x, y)$ of the operator A . Since

$$A = (-\Delta_\omega^D - E_1) \otimes 1 + 1 \otimes (-\partial_3^2 + \dot{\theta}^2),$$

we have

$$\exp(-tA)(x, y) = \sum_{j=1}^{\infty} e^{t(E_1 - E_j)} \psi_j(x_1, x_2) \psi_j(y_1, y_2) q(t, x_3, y_3), \quad (3.33)$$

where $q(t, r, s)$ is the heat kernel of the one-dimensional Schrödinger operator

$$-\frac{d^2}{dr^2} + \dot{\theta}^2(r) \quad \text{in } L^2(\mathbb{R}), \quad (3.34)$$

and E_j and ψ_j are the eigenvalues and (normalized) eigenfunctions of $-\Delta_\omega^D$. By Proposition A.1, see Appendix A (cf. [M84, Theorem 4.2]), there exists a positive constant c such that

$$q(t, r, r) \leq \frac{c g_0^2(r)}{t^{3/2}} \quad \text{if } t \geq 1, \quad q(t, r, r) \leq \frac{c}{\sqrt{t}} \quad \text{if } 0 < t < 1, \quad (3.35)$$

where g_0 is the function defined by (3.22). On the other hand, by the ultracontractivity of $e^{t\Delta_\omega^D}$ we have [D89, Theorem 4.2.5]

$$\sum_{j=1}^{\infty} e^{t(E_1 - E_j)} \psi_j^2(x_1, x_2) \leq c \psi_1^2(x_1, x_2) \quad t \geq 1. \quad (3.36)$$

Finally, by [D89, Theorem 4.6.2] we have

$$e^{t\Delta_\omega^D}((x_1, x_2), (x_1, x_2)) e^{tE_1} = \sum_{j=1}^{\infty} e^{t(E_1 - E_j)} \psi_j^2(x_1, x_2) \leq \frac{c}{t^2} \psi_1^2(x_1, x_2) \quad 0 < t < 1. \quad (3.37)$$

Combining all these estimates gives

$$e^{-tA}(x, x) \leq c \psi_1^2(x_1, x_2) g_0^2(x_3) \gamma(t) = c w_0^2(x) \gamma(t) \quad (3.38)$$

Next, mimicking the construction of the operator B_0 above we notice that the operator $\tilde{A}_0 := \mathcal{V}_0 A \mathcal{V}_0^{-1}$, where \mathcal{V}_0 is the unitary transformation $\mathcal{V}_0 : L^2(\Omega_0) \rightarrow L^2(\Omega_0, w_0^2)$ acting as

$$(\mathcal{V}_0 u)(x) := w_0^{-1}(x) u(x), \quad x \in \Omega_0, \quad (3.39)$$

is associated with the closed quadratic form

$$\tilde{Q}_0[f] := \int_{\Omega_0} |\nabla f|^2 w_0^2 dx, \quad f \in D(\tilde{Q}_0) = H^1(\Omega_0, w_0^2). \quad (3.40)$$

By (3.38) we then get

$$\sup_x e^{-t\tilde{A}_0}(x, x) = \sup_x \frac{e^{-tA}(x, x)}{w_0^2(x)} \leq c \gamma(t) \quad (3.41)$$

for all $t > 0$. Hence, in view of (4.2), we get

$$\|e^{-t\tilde{A}_0}\|_{L^1(\Omega_0, w_0^2) \rightarrow L^\infty(\Omega_0, w_0^2)} \leq m_\lambda(t) \quad (3.42)$$

if λ in (3.30) is chosen large enough. Note that $(-\log m_\lambda(t))'$ has a polynomial growth. Therefore, (3.42) and [Cou, Proposition II.4] yield

$$\xi_\lambda(\|f\|_{L^2(\Omega_0, w_0^2)}^2) \leq \int_{\Omega_0} |\nabla f|^2 w_0^2 dx \quad \forall f \in C_0^\infty(\Omega_0) : \|f\|_{L^1(\Omega_0, w_0^2)} \leq 1. \quad (3.43)$$

Hence (3.32) follows by density. \square

In a similar way as we introduced the functions m_λ and ξ_λ we define

$$\mu_\lambda(t) := \lambda \begin{cases} t^{-5/2}, & 0 < t \leq 1/2, \\ \tilde{\chi}(t), & 1/2 < t \leq 1, \\ t^{-1/2}, & 1 < t < \infty, \end{cases} \quad (3.44)$$

where $\tilde{\chi}$ is a C^1 decreasing convex function chosen such that $\mu_\lambda(t)$ is $C^1(\mathbb{R}_+)$. Accordingly, we define

$$\vartheta_\lambda(r) := -\mu'_\lambda(\mu_\lambda^{-1}(r)), \quad r \in \mathbb{R}_+. \quad (3.45)$$

Lemma 3.8. *There exist $\lambda_j > 0$, $j = 1, 2$, such that the inequality*

$$\vartheta_\lambda(\|f\|_{L^2(\Omega_0, w_j^2)}^2) \leq \int_{\Omega_0} |\nabla f|^2 w_j^2 dx, \quad j = 1, 2 \quad (3.46)$$

holds for all $f \in H^1(\Omega_0, w_j^2) \cap L^1(\Omega_0, w_j^2)$ with $\|f\|_{L^1(\Omega_0, w_j^2)} \leq 1$ and all $\lambda > \lambda_j$.

Proof. We introduce operators $\tilde{A}_j := \mathcal{V}_j A \mathcal{V}_j^{-1}$, where \mathcal{V}_j , $j = 1, 2$ are unitary transformations $\mathcal{V}_j : L^2(\Omega_0) \rightarrow L^2(\Omega_0, w_j^2)$ which act as

$$(\mathcal{V}_j u)(x) := w_j^{-1}(x) u(x), \quad x \in \Omega_0. \quad (3.47)$$

These operators are associated with closed quadratic forms

$$\tilde{Q}_j[f] := \int_{\Omega_0} |\nabla f|^2 w_j^2 dx, \quad f \in D(\tilde{Q}_j) = H^1(\Omega_0, w_j^2). \quad (3.48)$$

We follow the arguments of the proof of Lemma 3.7 replacing (3.35) by

$$q(t, r, r) \leq \frac{1}{\sqrt{4\pi t}} \leq \frac{c g_j^2(r)}{\sqrt{t}} \quad \forall t \geq 0,$$

which follows from Proposition A.1 given in Appendix A. This leads to

$$\sup_x e^{-t \tilde{A}_j}(x, x) = \sup_x \frac{e^{-t A}(x, x)}{w_j^2(x)} \leq c \Gamma(t), \quad j = 1, 2 \quad (3.49)$$

for all $t > 0$, and therefore, if λ in (3.44) is chosen large enough, then

$$\|e^{-t \tilde{A}_j}\|_{L^1(\Omega_0, w_j^2) \rightarrow L^\infty(\Omega_0, w_j^2)} \leq \mu_\lambda(t).$$

The statement then follows as in the proof of Lemma 3.7. \square

3.1.1. On-diagonal upper bounds. The functional inequalities proven in the previous Lemmata enable us to prove the following on-diagonal heat kernel estimates.

Proposition 3.9. *There exists a constant C such that for any $x \in \Omega_0$ and any $t > 0$ the following inequality holds:*

$$e^{-t H_\theta}(x, x) \leq C \psi_1^2(x_1, x_2) (1 + x_3^2) \gamma(t). \quad (3.50)$$

Proof. We note that $|\partial_\tau f|^2 \leq C_\omega |\nabla_\top f|^2$ for some constant C_ω . Using the inequality

$$2|\dot{\theta}| |\partial_3 f| |\partial_\tau f| \leq \varepsilon |\partial_3 f|^2 + \varepsilon^{-1} |\dot{\theta}|^2 |\partial_\tau f|^2, \quad 0 < \varepsilon < 1,$$

and taking ε close to 1, it is then easy to see that

$$|\nabla_\top f|^2 + |\partial_3 f + \dot{\theta} \partial_\tau f|^2 \geq c_0 |\nabla f|^2 \quad (3.51)$$

for some $c_0 > 0$. Let $\|f\|_{L^1(\Omega_0, v_0^2)} \leq 1$. By Lemma 3.6 we have $\kappa_0^{-1} \leq v_0^2/w_0^2 \leq \kappa_0$ for some $\kappa_0 > 1$. We apply Lemma 3.7 to the function $\tilde{f} := \kappa_0^{-1} f$. Using the fact that ξ_λ is increasing, in view of Lemma B.1, see appendix B, and (3.51) we obtain

$$\begin{aligned} \xi_\lambda(\|f\|_{L^2(\Omega_0, v_0^2)}^2) &\leq \xi_\lambda(\kappa_0^3 \|\tilde{f}\|_{L^2(\Omega_0, w_0^2)}^2) \leq C_{\kappa_0^3} \xi_\lambda(\|\tilde{f}\|_{L^2(\Omega_0, w_0^2)}^2) \\ &\leq C_{\kappa_0^3} \kappa_0^{-2} \int_{\Omega_0} |\nabla f|^2 w_0^2 dx \leq a_0^{-1} Q_0[f], \quad a_0 := c_0 \kappa_0 C_{\kappa_0^3}^{-1}, \end{aligned}$$

where c_0 is the constant in (3.51). Hence

$$a_0 \xi_\lambda(\|f\|_{L^2(\Omega_0, v_0^2)}^2) \leq Q_0[f] \quad \forall f \in C_0^\infty(\Omega_0) : \|f\|_{L^1(\Omega_0, v_0^2)} \leq 1. \quad (3.52)$$

This inequality extends by density to all functions $f \in H^1(\Omega_0, v_0^2)$ with $\|f\|_{L^1(\Omega_0, v_0^2)} \leq 1$. By the standard Beurling-Deny criteria and [D89, Thm.1.3.3] it follows that the operator B_0 associated with the form Q_0 generates a positivity preserving semigroup e^{-tB_0} which is contractive in $L^p(\Omega_0, v_0^2)$ for all $p \in [1, \infty]$ and all $t \geq 0$. These facts and the integrability at infinity of $1/\xi_\lambda$ (see Appendix B) allow us to apply [Cou, Proposition II.1] which, in view of (3.52), gives

$$\|e^{-tB_0}\|_{L^1(\Omega_0, v_0^2) \rightarrow L^\infty(\Omega_0, v_0^2)} \leq m_\lambda(a_0 t). \quad (3.53)$$

Equation (3.50) thus follows by applying (3.29). \square

Remark 3.10. As expected, the twisting influences the decay rate of $e^{-tH_\theta}(x, x)$ for large times. On the other hand, the faster decay in time is compensated by the additional weight factor $(1 + x_3^2)$. From our heat kernel lower bounds, see Theorem 3.15, it follows that the growth of this weight cannot be improved.

The next result holds for twisted as well as for straight tubes, i.e. for $\dot{\theta} \equiv 0$.

Proposition 3.11. *There exists a constant C such that for any $x \in \Omega_0$ and any $t > 0$*

$$e^{-tH_\theta}(x, x) \leq C \psi_1^2(x_1, x_2) \Gamma(t). \quad (3.54)$$

Proof. We define transformations $\mathcal{U}_j : L^2(\Omega_0) \rightarrow L^2(\Omega_0, v_j^2)$ by

$$(\mathcal{U}_j u)(x) := v_j^{-1}(x) u(x), \quad x \in \Omega_0, \quad j = 1, 2. \quad (3.55)$$

Hence \mathcal{U}_j map $L^2(\Omega_0)$ unitarily onto $L^2(\Omega_0, v_j^2)$ and $\mathcal{Q}[u]$ transforms into

$$Q_j[f] := \mathcal{Q}[v_j f] = \int_{\Omega_0} (|\nabla_\tau f|^2 + |\partial_3 f + \dot{\theta} \partial_\tau f|^2) v_j^2 dx, \quad f \in D(Q_j) = H^1(\Omega_0, w_j^2), \quad (3.56)$$

Accordingly, we introduce operators $B_j := \mathcal{U}_j H_\theta \mathcal{U}_j^{-1}$ generated by the quadratic forms Q_j . As above, we get

$$e^{-tH_\theta}(x, y) = v_j(x) v_j(y) e^{-tB_j}(x, y), \quad j = 1, 2. \quad (3.57)$$

In the same way as in the proof of Proposition 3.9 (using Lemma 3.8) we thus arrive at

$$\|e^{-tB_j}\|_{L^1(\Omega_0, v_j^2) \rightarrow L^\infty(\Omega_j, v_j^2)} \leq \mu_\lambda(a_j t), \quad j = 1, 2,$$

where $a_j > 0$. Hence by (3.57)

$$e^{-tH_\theta}(x, x) \leq c \psi_1^2(x_1, x_2) g_1^2(x_3) \Gamma(t), \quad e^{-tH_\theta}(x, x) \leq c \psi_1^2(x_1, x_2) g_2^2(x_3) \Gamma(t)$$

for all $x \in \Omega_0$ and $t > 0$. This concludes the proof. \square

Theorem 3.12. *There exists a constant $C > 0$ such that for any $\mathbf{x} \in \Omega$ and any $t \geq 1$ the following inequalities hold true*

$$k(t, \mathbf{x}, \mathbf{x}) \leq C \rho^2(\mathbf{x}) \min \left\{ (1 + \mathbf{x}_3^2) t^{-\frac{3}{2}}, t^{-\frac{1}{2}} \right\}. \quad (3.58)$$

Proof. Let $\mathbf{x}, \mathbf{y} \in \Omega$. From

$$U_\theta^{-1} e^{-tH_\theta} U_\theta = e^{t(\Delta_\Omega^D + E_1)}$$

we get

$$k(t, \mathbf{x}, \mathbf{y}) = e^{-tH_\theta} (r_\theta^{-1} \mathbf{x}, r_\theta^{-1} \mathbf{y}).$$

The statement thus follows directly from Propositions 3.9, 3.11 and Lemma 2.3. \square

3.1.2. Off-diagonal upper bounds. A combination of (3.2) with Theorem 3.12 gives

Corollary 3.13. *For any $C > 4$ there exists a constant $K_C > 0$ such that for any $\mathbf{x} \in \Omega$ and any $t \geq 1$ it holds*

$$k(t, \mathbf{x}, \mathbf{y}) \leq K_C \rho(\mathbf{x}) \rho(\mathbf{y}) \min \left\{ \sqrt{(1 + \mathbf{x}_3^2)(1 + \mathbf{y}_3^2)} t^{-\frac{3}{2}}, t^{-\frac{1}{2}} \right\} e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{Ct}}, \quad (3.59)$$

Proof. From (3.2) and Theorem 3.12 it follows that

$$k(t, \mathbf{x}, \mathbf{x}) \leq C \rho^2(\mathbf{x}) (1 + \mathbf{x}_3^2) \gamma(t) \quad \forall \mathbf{x} \in \Omega, \forall t > 0.$$

A direct inspection shows that [Gr97, Theorem 3.1] is applicable to $k(t, \mathbf{x}, \mathbf{y})$ with the respective functions f and g which parametrically depending on \mathbf{x} and \mathbf{y} (see the example in [Gr97, p. 37]). Hence for any $C > 4$ and all $t > 0$ it holds

$$k(t, \mathbf{x}, \mathbf{y}) \leq \delta(C) \rho(\mathbf{x}) \rho(\mathbf{y}) \sqrt{(1 + \mathbf{x}_3^2)(1 + \mathbf{y}_3^2)} \gamma(t) e^{-\frac{r(\mathbf{x}, \mathbf{y})^2}{Ct}}.$$

where $r(\mathbf{x}, \mathbf{y})$ is the geodesic distance between \mathbf{x} and \mathbf{y} and $\delta(C)$ is a positive constant which depends on C and $\gamma(\cdot)$. Repeating the same procedure with the bound

$$k(t, \mathbf{x}, \mathbf{x}) \leq C \rho^2(\mathbf{x}) \Gamma(t) \quad \forall \mathbf{x} \in \Omega, \forall t > 0,$$

which again follows from (3.2) and Theorem 3.12, we obtain

$$k(t, \mathbf{x}, \mathbf{y}) \leq \tilde{\delta}(C) \rho(\mathbf{x}) \rho(\mathbf{y}) \Gamma(t) e^{-\frac{r(\mathbf{x}, \mathbf{y})^2}{Ct}}.$$

The fact that $r(\mathbf{x}, \mathbf{y}) \geq |\mathbf{x} - \mathbf{y}|$ completes the proof. \square

Remark 3.14. By [Zh02], there exist positive constants c , C and T such that for any $\mathbf{x}, \mathbf{y} \in \Omega$ and any $0 < t \leq T$ the following off-diagonal estimates holds true

$$\min \left\{ \frac{\rho(\mathbf{x}) \rho(\mathbf{y})}{t}, 1 \right\} \frac{c e^{-\frac{C|\mathbf{x}-\mathbf{y}|^2}{t}}}{t^{3/2}} \leq k(t, \mathbf{x}, \mathbf{y}) \leq \min \left\{ \frac{\rho(\mathbf{x}) \rho(\mathbf{y})}{t}, 1 \right\} \frac{e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{Ct}}}{ct^{3/2}}. \quad (3.60)$$

3.2. Heat kernel lower bounds and the Brownian bridge reformulation. The aim of this section is to show that the long time decay rate $t^{-3/2}$ of the upper bound (3.50) is sharp. We have

Theorem 3.15. *There exists a positive constant c such that for any $\mathbf{x} \in \Omega$ and any $t \geq 1$ it holds*

$$k(t, \mathbf{x}, \mathbf{x}) \geq c \rho(\mathbf{x})^2 \min \left\{ (1 + \mathbf{x}_3^2) t^{-\frac{3}{2}}, t^{-\frac{1}{2}} \right\}. \quad (3.61)$$

Proof. We start by proving that for any $\mathbf{x} \in \Omega$ with $|x_3| > R + 1$ and any $t \geq 1$ we have

$$k(t, \mathbf{x}, \mathbf{x}) \geq C \rho(\mathbf{x})^2 t^{-\frac{1}{2}} \min \left\{ 1, \frac{\mathbf{x}_3^2}{t} \right\}, \quad C > 0. \quad (3.62)$$

Suppose that $\mathbf{x}_3 < -(R + 1)$. To get a lower bound on $k(t, \mathbf{x}, \mathbf{x})$ we impose additional Dirichlet boundary conditions at ω_{-R} , and denote by $\tilde{k}(t, \mathbf{x}, \mathbf{y})$ the heat kernel of the Laplacian on $\omega \times (-\infty, -R)$. In view of the reflection principle, see e.g. [D89, Section 4.1] and the ultracontractivity of $e^{t\Delta_\omega^D}$, we get

$$\begin{aligned} k(t, \mathbf{x}, \mathbf{y}) &\geq \tilde{k}(t, \mathbf{x}, \mathbf{y}) \\ &= \frac{1}{\sqrt{4\pi t}} \left(e^{-\frac{(\mathbf{x}_3 - \mathbf{y}_3)^2}{4t}} - e^{-\frac{(\mathbf{x}_3 + \mathbf{y}_3 + 2R)^2}{4t}} \right) \sum_{j \geq 1} e^{(E_1 - E_j)t} \psi_j(\mathbf{x}_1, \mathbf{x}_2) \psi_j(\mathbf{y}_1, \mathbf{y}_2) \\ &\geq C \frac{1}{\sqrt{4\pi t}} \left(e^{-\frac{(\mathbf{x}_3 - \mathbf{y}_3)^2}{4t}} - e^{-\frac{(\mathbf{x}_3 + \mathbf{y}_3 + 2R)^2}{4t}} \right) \psi_1(\mathbf{x}_1, \mathbf{x}_2) \psi_1(\mathbf{y}_1, \mathbf{y}_2) \end{aligned} \quad (3.63)$$

for all $\mathbf{y} \in \Omega$ with $\mathbf{y}_3 < -R - 1$. Using the inequality

$$1 - e^{-z} \geq (1 - e^{-1}) \min\{1, z\}, \quad z \geq 0 \quad (3.64)$$

we thus get

$$k(t, \mathbf{x}, \mathbf{x}) \geq c \frac{1 - e^{-1}}{\sqrt{4\pi}} \psi_1^2(\mathbf{x}_1, \mathbf{x}_2) t^{-\frac{1}{2}} \min \left\{ 1, \frac{(\mathbf{x}_3 + R)^2}{t} \right\}.$$

Taking into account Lemma 2.3 and the elementary inequality

$$(\mathbf{x}_3 + R)^2 \geq \left(\frac{\mathbf{x}_3}{R + 1} \right)^2 \quad \forall \mathbf{x}_3 < -R - 1,$$

we obtain (3.62) for $\mathbf{x}_3 < -R - 1$. The proof of the corresponding lower bound for $\mathbf{x}_3 > R + 1$ is completely analogous.

In order to treat the case $|x_3| \leq R + 1$, we fix a \mathbf{y}_0 such that $(\mathbf{y}_0)_3 < -(R + 1)$, and a number $\varepsilon < \min\{\rho^2(\mathbf{y}_0), 1\}/4$. We then use the semigroup property to get, for any $t > 1$:

$$\begin{aligned} k(t, \mathbf{x}, \mathbf{x}) &= \int_{\Omega \times \Omega} k\left(\frac{1}{3}, \mathbf{x}, \mathbf{y}\right) k\left(t - \frac{2}{3}, \mathbf{y}, \mathbf{z}\right) k\left(\frac{1}{3}, \mathbf{z}, \mathbf{x}\right) d\mathbf{y} d\mathbf{z} \\ &\geq \int_{B(\mathbf{y}_0, \varepsilon) \times B(\mathbf{y}_0, \varepsilon)} k\left(\frac{1}{3}, \mathbf{x}, \mathbf{y}\right) \tilde{k}\left(t - \frac{2}{3}, \mathbf{y}, \mathbf{z}\right) k\left(\frac{1}{3}, \mathbf{z}, \mathbf{x}\right) d\mathbf{y} d\mathbf{z}. \end{aligned}$$

To bound from below the terms involving the time $s = 1/3$, we use Zhang's off-diagonal lower bound (3.60). From the choice of \mathbf{y}_0 and ε and it follows that

$$k\left(\frac{1}{3}, \mathbf{x}, \mathbf{y}\right) \geq C_1(\mathbf{y}_0, \varepsilon) \rho(\mathbf{x}), \quad k\left(\frac{1}{3}, \mathbf{z}, \mathbf{x}\right) \geq C_2(\mathbf{y}_0, \varepsilon) \rho(\mathbf{x}), \quad \forall \mathbf{y}, \mathbf{z} \in B(\mathbf{y}_0, \varepsilon).$$

Here we used the fact that $|\mathbf{x} - \mathbf{y}|^2 + |\mathbf{x} - \mathbf{z}|^2$ is bounded from above since $|x_3| \leq R + 1$. Hence

$$k(t, \mathbf{x}, \mathbf{x}) \geq C \rho^2(\mathbf{x}) \int_{B(\mathbf{y}_0, \varepsilon) \times B(\mathbf{z}_0, \varepsilon)} \tilde{k}\left(t - \frac{2}{3}, \mathbf{y}, \mathbf{z}\right) d\mathbf{y} d\mathbf{z}$$

From (3.63) and (3.64) we get

$$\tilde{k}\left(t - \frac{2}{3}, \mathbf{y}, \mathbf{z}\right) \geq C t^{-\frac{1}{2}} \min\left\{1, \frac{1 + \mathbf{x}_3^2}{t}\right\} \quad \forall \mathbf{y}, \mathbf{z} \in B(\mathbf{y}_0, \varepsilon),$$

which concludes the proof. \square

Remark 3.16. In view of (3.62) it follows that the quadratic growth of the weight $(1 + \mathbf{x}_3^2)$ in (3.61) is sharp. The lower bound (3.62) holds also for $t \leq 1$. However, for small times the bounds (3.2) proved in [Zh02] are sharper.

It is also worth noticing that, because of a well-known probabilistic interpretation of the Dirichlet heat kernel, the above results can be reformulated in terms of the survival probability of the Brownian bridge killed upon exiting Ω . In fact we have the following nonstandard asymptotic result.

Corollary 3.17. *Let $\{X_s\}_{s \geq 0}$ be the Brownian loop process joining x to itself in time t and let $P^{t,x,x}$ be the conditional Wiener measure, normalized so that its total mass coincides with the free heat kernel on \mathbb{R}^3 . Then there exist strictly positive constants c_1, c_2 such that, for all $\mathbf{x} \in \Omega$:*

$$\begin{aligned} c_1 (1 + |\mathbf{x}_3|^2) \rho^2(\mathbf{x}) &\leq \liminf_{t \rightarrow +\infty} \left[t^{\frac{3}{2}} e^{E_1 t} P^{t,\mathbf{x},\mathbf{x}}(X_s \in \Omega \ \forall s \in [0, t]) \right] \\ &\leq \limsup_{t \rightarrow +\infty} \left[t^{\frac{3}{2}} e^{E_1 t} P^{t,\mathbf{x},\mathbf{x}}(X_s \in \Omega \ \forall s \in [0, t]) \right] \leq c_2 (1 + |\mathbf{x}_3|^2) \rho^2(\mathbf{x}). \end{aligned}$$

3.3. Generalization. As already mentioned in the Introduction, the method that we use to prove Theorem 3.1 is applicable to a wide class of operators in $L^2(\Omega_0)$. To be more specific, let us consider nonnegative uniformly elliptic operators of the form

$$L f = - \sum_{i,j=1}^3 \partial_{x_i} (a_{ij}(x) \partial_{x_j} f) + V(x) f, \quad (3.65)$$

where L is understood as the Friedrichs extension of the differential operator on the right hand side defined originally on $C_0^\infty(\Omega_0)$. We suppose that $a := (a_{ij})$ and V are sufficiently smooth in $\overline{\Omega_0}$ and that $L = -\Delta - E_1$ for $|x_3|$ large enough. The arguments in the proof of Theorem 3.15 then immediately give a lower bound on $e^{-tL}(x, x)$ given by the right hand side of (3.61) with \mathbf{x} replaced by x and $\rho(\mathbf{x})$ replaced by $\text{dist}(x, \partial\Omega_0)$.

On the other hand, if we also suppose that L is subcritical, then by Theorem 3.4 and [P88, Lemma 2.4] it follows that there exist smooth positive functions u_j , $j = 0, 1, 2$, such that $L u_j = 0$ in Ω_0 , and $u_j \asymp w_j$. Moreover, by the uniform ellipticity of L we have

$$(u_j \varphi, L(u_j \varphi))_{L^2(\Omega_0)} = \int_{\Omega_0} (\nabla \varphi \cdot (a \nabla \varphi)) u_j^2 dx \geq c \int_{\Omega_0} |\nabla \varphi|^2 w_j^2 dx,$$

for $j = 0, 1, 2$. Hence a straightforward modification of Propositions 3.9 and 3.11 gives

Theorem 3.18. *Let L be a uniformly elliptic operator of the form (3.65), and assume that a_{ij} and V are Hölder continuous in $\overline{\Omega_0}$, and that $L = -\Delta - E_1$ in $\{(x', x_3) \in \Omega_0 \mid |x_3| > R\}$ for some $R > 0$. Assume further that L is subcritical in Ω_0 . Then*

$$\exp(-tL)(x, x) \asymp \frac{\text{dist}(x, \partial\Omega_0)^2}{\sqrt{t}} \min\left\{\frac{1+x_3^2}{t}, 1\right\}, \quad \forall t \geq 1, \quad \forall x \in \Omega_0. \quad (3.66)$$

Large time behaviors of the heat kernel and in particular sharp two-sided heat kernel estimates are closely related to the following conjecture.

Conjecture 3.19 (Davies' Conjecture [D97]). *Consider a time independent second-order parabolic operator of the form*

$$u_t + P(x, \partial_x)u$$

which is defined on a noncompact Riemannian manifold M . Assume that $E_1 = E_1(P, M)$, the generalized principal eigenvalue of the elliptic operator P in M , is nonnegative. Let $k_P^M(x, y, t)$ be the corresponding positive minimal heat kernel. Fix reference points $x_0, y_0 \in M$.

Then

$$\lim_{t \rightarrow \infty} \frac{k_P^M(x, y, t)}{k_P^M(x_0, y_0, t)} = a(x, y) \quad (3.67)$$

exists and is positive for all $x, y \in M$ (see also [P06, FKP] and the references therein).

Recall that Davies' conjecture holds if $P - E_1$ is critical in M and the product of the corresponding ground states is in $L^1(M)$. Moreover, it holds true in the *symmetric* case if the cone of all positive solutions of the equation $(P - E_1)u = 0$ that vanish on ∂M is one-dimensional. Hence, it holds true for a critical symmetric operator. In particular,

$$\lim_{t \rightarrow \infty} \frac{e^{t\Delta_{\Omega_0}^D}(x, y)}{e^{t\Delta_{\Omega_0}^D}(0, 0)} = C\psi_1(x_1, x_2)\psi_1(y_1, y_2)$$

In the following remark we consider Davies' conjecture in the present situation.

Remark 3.20. It follows from [M84, Theorem 4.2] that Davies' conjecture holds true for Schrödinger operators on \mathbb{R} provided the potential satisfies Murata's assumptions in [M84]. Clearly,

$$\lim_{t \rightarrow \infty} \left(\sum_{j=1}^{\infty} e^{t(E_1 - E_j)} \psi_j(x_1, x_2) \psi_j(y_1, y_2) \right) = \psi_1(x_1, x_2) \psi_1(y_1, y_2). \quad (3.68)$$

Using the heat kernel decomposition (3.33), (3.68) and [M84, Theorem 4.2], it follows that Davies' conjecture holds true for the operator A on Ω_0 , where A is the subcritical operator defined by (3.5). The validity of Davies's conjecture for operators L satisfying the assumptions of Theorem 3.18 and for the Laplacian on a twisted tube remains open.

4. Integral estimates

In this section we will prove certain integral estimates for the semigroup $e^{t(\Delta_{\Omega}^D + E_1)}$. We start with a simple consequence of Theorem 3.12.

Corollary 4.1. *There exists a constant C such that for any $\mu, \nu \in [0, 1]$ and any $t \geq 1$ it holds*

$$k(t, \mathbf{x}, \mathbf{y}) \leq C \rho(\mathbf{x}) \rho(\mathbf{y}) (1 + \mathbf{x}_3^2)^{\frac{\mu}{2}} (1 + \mathbf{y}_3^2)^{\frac{\nu}{2}} t^{-\frac{1+\mu+\nu}{2}}. \quad (4.1)$$

Proof. We recall the following well-known inequality:

$$k(t, \mathbf{x}, \mathbf{y}) \leq \sqrt{k(t, \mathbf{x}, \mathbf{x})} \sqrt{k(t, \mathbf{y}, \mathbf{y})}. \quad (4.2)$$

For the convenience of the reader we briefly recall the proof of this fact. By the semigroup property and the symmetry of the heat kernel

$$k(2t, \mathbf{x}, \mathbf{x}) = \int_{\Omega} k(t, \mathbf{x}, \mathbf{y})^2 d\mathbf{y}. \quad (4.3)$$

Hence, again by the semigroup property and Cauchy–Schwarz we get

$$\begin{aligned} k(2t, \mathbf{x}, \mathbf{y}) &= \int_{\Omega} k(t, \mathbf{x}, \mathbf{z}) k(t, \mathbf{y}, \mathbf{z}) d\mathbf{z} \leq \left(\int_{\Omega} k(t, \mathbf{x}, \mathbf{z})^2 d\mathbf{z} \right)^{1/2} \left(\int_{\Omega} k(t, \mathbf{y}, \mathbf{z})^2 d\mathbf{z} \right)^{1/2} \\ &= k(2t, \mathbf{x}, \mathbf{x})^{1/2} k(2t, \mathbf{y}, \mathbf{y})^{1/2} \end{aligned} \quad (4.4)$$

as claimed. It now remains to apply Proposition 3.11 and Theorem 3.12. \square

Now let us introduce the following family of weighted L^p spaces:

$$L_{\beta}^p(\Omega) := \left\{ f : \|f\|_{L_{\beta}^p(\Omega)} < \infty \right\}, \quad \|f\|_{L_{\beta}^p(\Omega)} := \left(\int_{\Omega} |f|^p (1 + \mathbf{x}_3^2)^{\beta} d\mathbf{x} \right)^{\frac{1}{p}}, \quad \beta \in \mathbb{R}.$$

With this notation we have

Proposition 4.2. *For any $\kappa \in [0, 2]$ and any $\beta > (1 + \kappa)/2$ there exists $C = C(\beta, \kappa)$ such that*

$$\|e^{t(\Delta_{\Omega}^D + E_1)}\|_{L_{\beta}^2(\Omega) \rightarrow L^2(\Omega)} \leq C(1+t)^{-\frac{1+\kappa}{4}} \quad \forall t \geq 0. \quad (4.5)$$

Proof. Let $f \in L^2(\Omega)$. In view of (4.3), Cauchy–Schwarz inequality and (4.1) applied with $\mu = \nu = \kappa/2$ we get

$$\begin{aligned} \|e^{t(\Delta_{\Omega}^D + E_1)} f\|_{L^2(\Omega)}^2 &\leq \|f\|_{L_{\beta}^2(\Omega)}^2 \int_{\Omega \times \Omega} k(t, \mathbf{x}, \mathbf{y})^2 (1 + \mathbf{y}_3^2)^{-\beta} d\mathbf{x} d\mathbf{y} \\ &= \|f\|_{L_{\beta}^2(\Omega)}^2 \int_{\Omega} k(2t, \mathbf{y}, \mathbf{y}) (1 + \mathbf{y}_3^2)^{-\beta} d\mathbf{y} \leq \tilde{C} t^{-\frac{1+\kappa}{2}} \|f\|_{L_{\beta}^2(\Omega)}^2 \end{aligned}$$

for all $t \geq 1$. This shows that

$$\|e^{t(\Delta_{\Omega}^D + E_1)}\|_{L_{\beta}^2(\Omega) \rightarrow L^2(\Omega)} \leq C t^{-\frac{1+\kappa}{4}} \quad \forall t \geq 1. \quad (4.6)$$

Equation (4.5) then follows from (4.6) and from the fact that $e^{t(\Delta_{\Omega}^D + E_1)}$ is, for all $t \geq 0$, a contraction from $L^2(\Omega)$ to $L^2(\Omega)$. \square

Remark 4.3. Proposition 4.2 with $\kappa = 2$ extends inequality (1.5) to any $L_{\beta}^2(\Omega)$ with $\beta > 3/2$. On the other hand, the corresponding estimate in [KZ10] was obtained under weaker regularity assumptions on θ .

The following estimate is a version of Proposition 4.2 in suitable L^1 and L^{∞} spaces. In order to state it we introduce for $\beta \geq 0$ the spaces

$$L_{-\beta}^{\infty}(\Omega) = \left\{ f : \|f\|_{L_{-\beta}^{\infty}(\Omega)} := \|(1 + \mathbf{x}_3^2)^{-\beta} f\|_{L^{\infty}(\Omega)} < \infty \right\}.$$

We then have

Theorem 4.4. *For any $\beta \in [0, 1/2]$ we have*

$$\|e^{t(\Delta_\Omega^D + E_1)}\|_{L^2(\Omega) \rightarrow L^\infty_\beta(\Omega)} = \|e^{t(\Delta_\Omega^D + E_1)}\|_{L^1_\beta(\Omega) \rightarrow L^2(\Omega)} \asymp t^{-\frac{1}{4}-\beta} \quad \forall t \geq 1. \quad (4.7)$$

Proof. The equality in (4.7) follows by duality using the scalar product $(u, v) = \int_\Omega \bar{u}v \, d\mathbf{x}$ in $L^2(\Omega)$. Let $f \in L^2(\Omega)$. By (4.3), Cauchy-Schwarz inequality and estimate (4.1) with $\mu = \nu = 2\beta$ we obtain

$$\begin{aligned} \|e^{t(\Delta_\Omega^D + E_1)} f\|_{L^\infty_\beta(\Omega)} &\leq \|f\|_{L^2(\Omega)} \|(1 + \mathbf{x}_3^2)^{-\beta} \sqrt{k(2t, \mathbf{x}, \mathbf{x})}\|_{L^\infty(\Omega)} \\ &\leq C_\beta t^{-\frac{1}{4}-\beta} \|f\|_{L^2(\Omega)}. \end{aligned}$$

This proves the upper bound in (4.7). To prove the lower bound let us consider a generalized function f_t given by a Dirac delta distribution placed in a point $\mathbf{z}(t) \in \Omega$ such that $1 + \mathbf{z}_3^2(t) = 2t$ and $\rho(\mathbf{z}(t)) > \varepsilon > 0$ for all t . From (3.61) and (4.3) it then follows that

$$\frac{\|e^{t(\Delta_\Omega^D + E_1)} f_t\|_{L^2(\Omega)}}{\|f_t\|_{L^1_\beta(\Omega)}} = \frac{\sqrt{k(2t, \mathbf{z}(t), \mathbf{z}(t))}}{(1 + \mathbf{z}_3^2(t))^\beta} \geq C t^{-\frac{1}{4}-\beta}.$$

□

Remark 4.5. In the absence of twisting we have

$$\|e^{t(\Delta_{\Omega_0}^D + E_1)}\|_{L^2(\Omega_0) \rightarrow L^\infty_\beta(\Omega_0)} = \|e^{t(\Delta_{\Omega_0}^D + E_1)}\|_{L^1_\beta(\Omega_0) \rightarrow L^2(\Omega_0)} \asymp t^{-\frac{1}{4}} \quad \forall t \geq 1, \quad \forall \beta \geq 0,$$

which can be easily derived from the explicit expression for the integral kernel of $e^{t(\Delta_{\Omega_0}^D + E_1)}$ in Ω_0 . Notice also that proceeding as in the proof of Theorem 4.4 but choosing $\mathbf{z}(t) = \text{constant}$ shows that no matter how large β is, the left hand side of (4.7) will never decay faster than $t^{-\frac{3}{4}}$.

5. Spectral estimates and Sobolev inequality

Let $V : \Omega \rightarrow \mathbb{R}$ be a real valued measurable function and consider the Schrödinger operator

$$-\Delta_\Omega^D - V \quad \text{in } L^2(\Omega)$$

associated with the quadratic form

$$\int_\Omega (|\nabla u|^2 - V|u|^2) \, d\mathbf{x}, \quad u \in H_0^1(\Omega). \quad (5.1)$$

Let us denote by $N(-\Delta_\Omega^D - V, s)$ the number of discrete eigenvalues of $-\Delta_\Omega^D - V$ less than s (counted with multiplicity). If $V = 0$, then of course $N(-\Delta_\Omega^D, E_1) = 0$. In the problems concerning spectral estimates one usually tries to control $N(-\Delta_\Omega^D - V, E_1)$ in terms of V .

Without loss of generality we may assume that $V \geq 0$ (otherwise we replace V by V_+). By the Lieb's inequality, see [L, FLS, RS98], we have

$$\begin{aligned} N(-\Delta_\Omega^D - V, E_1) &= N(-\Delta_\Omega^D - E_1 - V, 0) \\ &\leq M_b \int_\Omega \int_0^\infty k(t, \mathbf{x}, \mathbf{x}) t^{-1} (tV(\mathbf{x}) - b)_+ \, dt \, d\mathbf{x}, \end{aligned} \quad (5.2)$$

where $b > 0$ is arbitrary and

$$M_b = (e^{-b} - b \int_b^\infty s^{-1} e^{-s} \, ds)^{-1}.$$

From inequality (3.2) and Theorem 3.12 follows that there exists a constant C such that for all $t > 0$ and all $\mathbf{x} \in \Omega$ it holds

$$k(t, \mathbf{x}, \mathbf{x}) \leq C (1 + \mathbf{x}_3^2) t^{-\frac{3}{2}}. \quad (5.3)$$

A direct application of (5.3) and (5.2) then gives

Theorem 5.1. *There exists a positive constant L such that*

$$N(-\Delta_\Omega^D - V, E_1) \leq L \int_\Omega V^{\frac{3}{2}}(\mathbf{x}) (1 + \mathbf{x}_3^2) d\mathbf{x} \quad (5.4)$$

holds for all $0 \leq V \in L^{3/2}(\Omega, (1 + \mathbf{x}_3^2))$.

Remark 5.2. Due to the criticality of $-\Delta_{\Omega_0}^D - E_1$, inequality (5.4) fails in the absence of twisting since

$$N(-\Delta_{\Omega_0}^D - \alpha V, E_1) \geq 1 \quad \forall \alpha > 0$$

provided $V \not\equiv 0$ satisfies the assumptions of Theorem 5.1, see [EW, PT06, RS09]. Note also that the bound (5.4) has the right semiclassical behavior since it is well-known, see e.g. [RS09] that

$$N(-\Delta_\Omega^D - \alpha V, E_1) \asymp \alpha^{3/2} \quad \alpha \rightarrow \infty.$$

Remark 5.3. It is also easy to see that the weight $(1 + \mathbf{x}_3^2)$ in (5.4) cannot be improved in the power-like scale. For if $V(\mathbf{x}) \asymp |\mathbf{x}_3|^{-2+\varepsilon}$ as $|\mathbf{x}| \rightarrow \infty$ with some $\varepsilon > 0$, then a standard test function argument, cf. [RS, Theorem 13.6], shows that

$$N(-\Delta_{\Omega_0}^D - \alpha V, E_1) = \infty \quad \forall \alpha > 0.$$

Estimate (5.4) in combination with Hardy inequality (1.3) yield the following family of weighted Sobolev inequalities, which have no analogue in the straight tube Ω_0 .

Theorem 5.4. *For any $p \in [2, 6]$ there exists a constant $C_p > 0$ such that*

$$\int_\Omega (|\nabla u|^2 - E_1 |u|^2) d\mathbf{x} \geq C_p \left(\int_\Omega |u|^p (1 + \mathbf{x}_3^2)^{-\frac{p+2}{4}} d\mathbf{x} \right)^{2/p} \quad (5.5)$$

holds for all $u \in H_0^1(\Omega)$.

Proof. First we mimic the argument used in [FLS] and note that by (5.4)

$$L \int_\Omega V^{3/2}(\mathbf{x}) (1 + \mathbf{x}_3^2) d\mathbf{x} < 1 \quad (5.6)$$

\Downarrow

$$\int_\Omega (|\nabla u|^2 - E_1 |u|^2 - V |u|^2) d\mathbf{x} \geq 0 \quad \forall u \in H_0^1(\Omega). \quad (5.7)$$

Let $u \in H_0^1(\Omega)$. Choosing

$$V(\mathbf{x}) = \eta |u|^4 (1 + \mathbf{x}_3^2)^{-2} \left(L \int_\Omega |u|^6 (1 + \mathbf{x}_3^2)^{-2} d\mathbf{x} \right)^{-\frac{2}{3}}$$

with $\eta < 1$ we see that (5.6) is satisfied and (5.7) gives

$$\int_\Omega (|\nabla u|^2 - E_1 |u|^2) d\mathbf{x} \geq C \left(\int_\Omega |u|^6 (1 + \mathbf{x}_3^2)^{-2} d\mathbf{x} \right)^{1/3}$$

for some $C > 0$. This together with Hölder inequality and (1.3) implies

$$\begin{aligned} \int_{\Omega} |u|^p (1 + \mathbf{x}_3^2)^{-\frac{p+2}{4}} d\mathbf{x} &\leq \left(\int_{\Omega} |u|^6 (1 + \mathbf{x}_3^2)^{-2} d\mathbf{x} \right)^{\frac{p-2}{4}} \left(\int_{\Omega} |u|^2 (1 + \mathbf{x}_3^2)^{-1} d\mathbf{x} \right)^{\frac{6-p}{4}} \\ &\leq c \left(\int_{\Omega} (|\nabla u|^2 - E_1 |u|^2) d\mathbf{x} \right)^{\frac{p}{2}}, \end{aligned}$$

as claimed. \square

Let us define the sequence of functions $g_n : \mathbb{R} \rightarrow \mathbb{R}$ by

$$g_n(s) := \begin{cases} 1 - \frac{1}{n}(s + R), & -R - n \leq s < -R, \\ 1, & -R \leq s \leq R, \\ 1 - \frac{1}{n}(s - R), & R < s < R + n, \end{cases}$$

and $g_n = 0$ otherwise, recalling that $\text{supp } \dot{\theta} \subset (-R, R)$. We make the following observations.

Remark 5.5. Due to the criticality of $-\Delta_{\Omega_0}^D - E_1$, inequality (5.5) fails if $\dot{\theta} \equiv 0$ [PT09]. Indeed, the choice $u_n(x) = \psi_1(x_1, x_2) g_n(x_3)$ gives $u_n \in H_0^1(\Omega_0)$ and

$$\int_{\Omega_0} (|\nabla u_n|^2 - E_1 |u_n|^2) dx = \int_{\mathbb{R}} |g'_n(x_3)|^2 dx_3 = \mathcal{O}(n^{-1}) \quad n \rightarrow \infty,$$

while

$$\int_{\Omega_0} |u_n|^p (1 + x_3^2)^{-\frac{p+2}{4}} dx \rightarrow \int_{\mathbb{R}} (1 + x_3^2)^{-\frac{p+2}{4}} dx_3 \quad n \rightarrow \infty$$

by monotone convergence theorem. This will be in contradiction with (5.5) if we replace Ω with Ω_0 .

Remark 5.6. The decay rate of the weight in the integral on the right hand side of (5.5) cannot be improved in the power-like scale. In other words the inequality

$$\int_{\Omega} (|\nabla u|^2 - E_1 |u|^2) d\mathbf{x} \geq C \left(\int_{\Omega} |u|^p (1 + \mathbf{x}_3^2)^{-\gamma} d\mathbf{x} \right)^{\frac{2}{p}} \quad \forall u \in H_0^1(\Omega) \quad (5.8)$$

fails whenever $\gamma < (p+2)/4$. To see this we use the sequence of test functions $u_n(\mathbf{x}) = v_0(r_{\theta}^{-1}\mathbf{x}) g_n(\mathbf{x}_3)$. Then $u_n \in H_0^1(\Omega)$ and using (3.26) we get

$$\int_{\Omega} (|\nabla u_n|^2 - E_1 |u_n|^2) d\mathbf{x} \leq C \int_{\mathbb{R}} (1 + \mathbf{x}_3^2) |g'_n(\mathbf{x}_3)|^2 d\mathbf{x}_3 = \mathcal{O}(n),$$

and

$$\left(\int_{\Omega} |u_n|^p (1 + \mathbf{x}_3^2)^{-\gamma} d\mathbf{x} \right)^{\frac{2}{p}} \geq C n^{\frac{2(p+1-2\gamma)}{p}} + o(n^{\frac{2(p+1-2\gamma)}{p}})$$

as $n \rightarrow \infty$. Hence from (5.8) it follows that $\gamma \geq (p+2)/4$.

APPENDIX A. **One-dimensional Schrödinger operators**

In this section we prove an auxiliary result concerning the semigroup generated by the nonnegative operator

$$P = -\frac{d^2}{dr^2} + \theta^2(r) \quad \text{in } L^2(\mathbb{R}).$$

Proposition A.1 (cf. [M84, Theorem 4.2]). *There exists a constant c such that*

$$q(t, r, r) := e^{-tP}(r, r) \leq c \min \left\{ \frac{g_0^2(r)}{t^{3/2}}, \frac{1}{\sqrt{t}} \right\} \quad \forall t > 0, \quad (\text{A.1})$$

where g_0 is given by (3.22).

Proof. One estimate follows immediately by the Trotter product formula:

$$e^{-tP}(r, r) \leq \exp \left(t \frac{d^2}{dr^2} \right) (r, r) = (4\pi t)^{-1/2}.$$

To prove the remaining part of (A.1) we note that since $Pg_0 = 0$, the operator $\tilde{P} := g_0^{-1} P g_0$ in $L^2(\mathbb{R}, g_0^2(r) dr)$ is associated with the quadratic form

$$\int_{\mathbb{R}} |f'(r)|^2 g_0^2(r) dr, \quad f \in H^1(\mathbb{R}, g_0^2(r) dr),$$

and the corresponding semigroup $e^{-t\tilde{P}}$ satisfies

$$e^{-tP}(r, r') = g_0(r) g_0(r') e^{-t\tilde{P}}(r, r').$$

Hence it suffices to show that

$$\sup_{r>0} e^{-t\tilde{P}}(r, r) \leq c t^{-3/2} \quad \forall t > 0. \quad (\text{A.2})$$

By the well-known Theorem of Varopoulos, see e.g. [D89, Theorem 2.4.2], estimate (A.2) will follow from the Sobolev inequality

$$\int_{\mathbb{R}} |f'(r)|^2 g_0^2(r) dr \geq c_s \left(\int_{\mathbb{R}} |f(r)|^6 g_0^2(r) dr \right)^{1/3} \quad \forall f \in H^1(\mathbb{R}, g_0^2(r) dr). \quad (\text{A.3})$$

To prove (A.3) we consider a function $u \in H^1(\mathbb{R}_+, (1+r)^2 dr)$. Integration by parts yields the identity

$$\int_0^\infty \left(u' + \frac{u}{2(1+r)} \right)^2 (1+r)^2 dr = \int_0^\infty |u'|^2 (1+r)^2 dr - \frac{u^2(0)}{2} - \frac{1}{4} \int_0^\infty |u|^2 dr. \quad (\text{A.4})$$

Moreover,

$$|u(r)|^2 = -2 \int_r^\infty u'(s) u(s) ds \leq \int_0^\infty |u'(r)|^2 dr + \int_0^\infty |u(r)|^2 dr.$$

This in combination with (A.4) and the Hölder inequality gives

$$\begin{aligned} \int_0^\infty |u'|^2 (1+r)^2 dr &\geq \frac{1}{8} \int_0^\infty |u'|^2 dr + \frac{1}{2} \int_0^\infty |u'|^2 (1+r)^2 dr \\ &\geq \frac{1}{8} \int_0^\infty |u'|^2 dr + \frac{1}{8} \int_0^\infty |u|^2 dr \geq \frac{1}{8} \|u\|_\infty^2 \geq \frac{1}{8} \left(\int_0^1 |u|^6 dr \right)^{1/3}. \end{aligned} \quad (\text{A.5})$$

On the other hand, restriction of the standard Sobolev inequality in \mathbb{R}^3 with the critical exponent $q = 6$ onto the subspace of radial functions gives

$$\int_0^\infty |u'|^2 r^2 dr \geq \tilde{c} \left(\int_0^\infty |u|^6 r^2 dr \right)^{1/3}. \quad (\text{A.6})$$

Hence inequality (A.3) follows from (A.5), (A.6) and from the fact that $g_0^2(r) \asymp (1 + |r|)^2 \asymp 1 + r^2$ on \mathbb{R} . \square

APPENDIX B. Properties of the functions ξ_λ and ϑ_λ

Lemma B.1. *Let ξ, ϑ be the functions defined by (3.31), (3.45). For any $\kappa > 0$ there exists a constant c_κ such that for all $r > 0$ and all $\lambda \geq 1$ it holds*

$$\xi_\lambda(\kappa r) \leq C_\kappa \xi_\lambda(r), \quad \vartheta_\lambda(\kappa r) \leq C_\kappa \vartheta_\lambda(r). \quad (\text{B.1})$$

Proof. Since ξ_λ is increasing, we may assume that $\kappa > 1$. A straightforward calculation gives

$$\xi_\lambda(r) = \begin{cases} \frac{3}{2} \lambda^{-\frac{2}{3}} r^{\frac{5}{3}}, & 0 < r \leq \lambda, \\ -\lambda \chi'(\chi^{-1}(r/\lambda)), & \lambda < r < 2^{\frac{5}{2}} \lambda, \\ \frac{5}{2} \lambda^{-\frac{2}{5}} r^{\frac{7}{5}}, & 2^{\frac{5}{2}} \lambda \leq r < \infty, \end{cases}$$

and

$$\vartheta_\lambda(r) = \begin{cases} \frac{1}{2} \lambda^{-2} r^3, & 0 < r \leq \lambda, \\ -\lambda \tilde{\chi}'(\tilde{\chi}^{-1}(r/\lambda)), & \lambda < r < 2^{\frac{5}{2}} \lambda, \\ \frac{5}{2} \lambda^{-\frac{2}{5}} r^{\frac{7}{5}}, & 2^{\frac{5}{2}} \lambda \leq r < \infty. \end{cases}$$

It can be now directly verified that ξ_λ and ϑ_λ satisfy (B.1). \square

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